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Some Multi-Material Closure Models for 1-D Lagrangian Hydrodynamics

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Overview

- **Lagrangian hydrodynamics of two materials in 1-D**
  - Two material, one-velocity model leads to a closure problem.
- **Three different staggered-mesh discretizations**
  - The approaches used in computations are presented.
- **Several different closure models**
  - All use pressure relaxation in the mixed cell as a physically-motivated assumption.
- **Comparison of computational results**
  - Pressure equilibration behavior for two test problems
- **Summary and conclusions**

"Das Ziel der Wissenschaft ist einerseits, neue Tatsachen zu erobern, andrerseits, bekannte unter höheren Gesichtspunkten zusammenzufassen."
Sophus Lie, *Gesammelte Abhandlungen*, B.G.Teubner, Leipzig, 1934.

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Two-material Lagrangian hydrodynamics in 1-D presents several open issues.

- **Conservation laws govern the flow of inviscid, non-heat-conducting, compressible fluids in the Lagrangian frame:**

Mass: $$\rho^0 \frac{D\tau}{Dt} - \frac{\partial u}{\partial x} = 0 \qquad \tau \equiv 1/\rho$$

Momentum: $$\rho^0 \frac{Du}{Dt} + \frac{\partial P}{\partial x} = 0 \qquad \rho^0 = \rho^0(x) \equiv \rho(x, t=0)$$

Energy: $$\rho^0 \frac{De}{Dt} + \frac{\partial}{\partial x}(Pu) = 0 \qquad e \equiv \varepsilon + (1/2)\,u^2$$

Equation of State (EOS): $$P = \mathcal{P}(\varepsilon, \tau)$$

Specific Internal Energy (SIE)

- **With 1-D equations, we <u>can</u>:**
  - Test — *rigorously* — fundamental algorithms
  - Quantitatively evaluate algorithm performance
- **With 1-D models, we <u>cannot</u> necessarily extend to 2-D.**

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We make some simplifying assumptions.

- **There are two materials.**
  - Two materials cells (almost) certainly occur during the remap of a multi-material ALE calculation.
  - Modeling of two materials requires much more care than one material simulations.
  - Modeling of two materials does not imply an unambiguous method for model three (or more) materials.
- **These two materials are described by one velocity.**
  - This implies — either implicitly or explicitly — that a sub-grid model describes the mixing of the materials within each cell.
  - This differs from more sophisticated, multiple velocity-field models that are used, e.g., for two-phase flow.
- **We focus on closure models for pressure equilibration.**
  - We do not discuss here the important issue of artificial viscosity models for multiple-material cells.*

* See: Yanilkin, Yu.V., *Study and Implementation of Multi-Material Pressure Relaxation Methods for Lagrangian Hydrodynamics*, Los Alamos National Laboratory report LA-UR-10-06664, 2010.

Algorithm I uses the following predictor-corrector approach*.

Predictor

Edge positions: $x_{i+1/2}^{n+1,*} = x_{i+1/2}^{n} + \Delta t \cdot u_{i+1/2}$

Cell volumes: $V_{i,\text{cell}}^{n+1,*} = x_{i+1/2}^{n+1,*} - x_{i-1/2}^{n+1,*}$

Edge-velocities: $u_{i+1/2}^{n+1,*} = u_{i+1/2}^{n} - \Delta t(p_{i+1}^{n} + q_{i+1}^{n} - p_{i}^{n} - q_{i}^{n}) \Big/ M_{i+1/2,\text{node}}^{n}$

Artificial viscosity

Cell pressure: $p_i^{n+1,*} = p_i^n - \chi\ \Delta t\ \rho_i^n\ (c_{s,i}^{n+1,*})^2\ \nabla \cdot u_i^n$

Adiabatic update

Corrector

Node mass: $M_{i+1/2,\text{node}} = \frac{1}{2}(M_{i,\text{cell}} + M_{i+1,\text{cell}})$

Edge-velocities: $u_{i+1/2}^{n+1} = u_{i+1/2}^{n} - \frac{\Delta t}{2}(p_{i+1}^{n+1,*} + q_{i+1}^{n+1,*} - p_i^{n+1,*} - q_i^{n+1,*} + p_{i+1}^{n} + q_{i+1}^{n} - p_i^{n} - q_i^{n}) \Big/ M_{i+1/2,\text{node}}$

Time-center: $u_{i+1/2}^{n+1/2} = \frac{1}{2}(u_{i+1/2}^{n} + u_{i+1/2}^{n+1})$

Edge positions: $x_{i+1/2}^{n+1} = x_{i+1/2}^{n} + \Delta t \cdot u_{i+1/2}^{n+1/2}$

Cell volumes: $V_{i,\text{cell}}^{n+1} = x_{i+1/2}^{n+1} - x_{i-1/2}^{n+1}$

Cell density.: $\rho_i^{n+1} = M_{i,\text{cell}} \Big/ V_{i,\text{cell}}^{n+1} \Rightarrow \tau_i^{n+1} = 1 \Big/ \rho_i^{n+1}$

Cell SIE: $\varepsilon_i^{n+1} = \varepsilon_i^{n} - (\Delta t / \rho_i^{n})(p_i^{n+1,*} + q_i^{n+1,*}) \left((V_{i+1/2}^{n+1} - V_{i+1/2}^{n}) \Big/ (\Delta t\ V_{i+1/2}^{n+1}) \right)$

Cell pressure: $p_i^{n+1} = \mathcal{P}(\varepsilon_i^{n+1}, \tau_i^{n+1})$ **Full EOS call**

* Yanilkin, Yu.V., *Study and Implementation of Multi-Material Pressure Relaxation Methods for Lagrangian Hydrodynamics*, Los Alamos National Laboratory report LA-UR-10-06664, 2010.

This algorithm changes for multiple materials.

- **Denote the volume fraction of material α as:** $f_\alpha = V_\alpha / V$
- **In the predictor, the change is to the pressure update.**
  - The pressure of material α at t^n is evaluated: $p^n_{i,\alpha} = \mathcal{P}(\varepsilon^n_{i,\alpha}, \tau^n_{i,\alpha})$
  - Pressure predictor update: $p^{n+1,*}_{i,\alpha} = p^n_{i,\alpha} - \chi\, \Delta t\, \rho^n_{i,\alpha} (c^n_{s,i,\alpha})^2\, \nabla \cdot u^n_i$
  - With the following relations, Bondarenko & Yanilkin* showed that total energy is conserved in this approach:

$$p^{n+1,*}_i = \sum_\alpha \psi_\alpha\, p^{n+1,*}_{i,\alpha} \qquad q^{n+1,*}_i = \sum_\alpha \psi_\alpha\, q^{n+1,*}_{i,\alpha}$$

    where ψ_α is determined by the closure model.

- **In the corrector, additional modifications are required.**
  - The node mass becomes:

$$M_{i+1/2,\text{node}} = \frac{1}{2} \sum_\alpha (M_{i,\alpha} + M_{i+1,\alpha}) \quad \text{where} \quad M_{i,\alpha} \equiv f_{i,\alpha}\, \rho_{i,\alpha}\, V_i$$

* Bondarenko, Yu.A., Yanilkin, Yu.V., "Computation of thermodynamical parameters of the mixed cells in gas dynamics," *VANT* (*Mathematical Modeling of Physical Processes*) 2000;**4**:12–25 (in Russian).

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Additional changes in the corrector are needed.

- **Updated values for material α are as follows:**

Volume: $$V_{i,\alpha}^{n+1} = V_{i,\alpha}^{n} + \Delta t\, V_{i,\alpha}^{n+1} \nabla\cdot u_{i,\alpha}^{n+1}$$

Density: $$\rho_{i,\alpha}^{n+1} = M_{i,\mathrm{cell},\alpha} \Big/ V_{i,\alpha}^{n+1} \quad \Rightarrow \quad \tau_{i,\alpha}^{n+1} = 1 \Big/ \rho_{i,\alpha}^{n+1}$$

Volume Fraction: $$f_{i,\alpha}^{n+1} = V_{i,\alpha}^{n+1} \Big/ V_{i}^{n+1}$$

SIE: $$\varepsilon_{i,\alpha}^{n+1} = \varepsilon_{i,\alpha}^{n} - (\Delta t \Big/ \rho_{i,\alpha}^{n})\,(p_{i,\alpha}^{n+1,*} + q_{i,\alpha}^{n+1,*}) \times (1/2)\,(\nabla\cdot u_{i,\alpha}^{n} + \nabla\cdot u_{i,\alpha}^{n+1,*})$$

  - In the above expressions, the following quantities are still undefined: artificial viscosity $q_{i,\alpha}^{n}$, velocity divergence $\nabla\cdot u_{i,\alpha}^{n}$, parameter ψ_α

- **We impose the following constraints:**

(1) Volume: $V = \sum_\alpha V_\alpha \Rightarrow \sum_\alpha f_\alpha = 1$ and $\Delta V = \sum_\alpha \delta V_\alpha$, $\sum_\alpha f_\alpha \nabla\cdot u_\alpha = \nabla\cdot u$

(2) SIE: $\varepsilon = \sum_\alpha Y_\alpha \varepsilon_\alpha$ with $Y_\alpha \equiv f_\alpha \rho_\alpha / \rho$, $\rho = \sum_\alpha f_\alpha \rho_\alpha$

- **Assume velocity divergence is modeled as:** $\nabla\cdot u_\alpha \equiv \lambda_\alpha \nabla\cdot u$ **such that** $\psi_\alpha \equiv f_\alpha \lambda_\alpha$

Algorithm II uses the following approach*.

Node mass: $M_{i+1/2,\text{node}} = (1/2)(M_{i,\text{cell}} + M_{i+1,\text{cell}})$

Time steps: $\Delta t^{+} \equiv t^{n+1} - t^{n}, \qquad \Delta t^{-} \equiv t^{n} - t^{n-1}$

Edge-velocities: $u_{i+1/2}^{n+1/2} = u_{i+1/2}^{n-1/2} - (1/2)(\Delta t^{+} + \Delta t^{-})(p_{i+1}^{n} + q_{i+1}^{n} - p_{i}^{n} - q_{i}^{n}) / M_{i+1/2,\text{node}}$

Edge positions: $x_{i+1/2}^{n+1} = x_{i+1/2}^{n} + \Delta t^{+} \cdot u_{i+1/2}^{n+1/2}$

Cell volumes: $V_{i,\text{cell}}^{n+1} = x_{i+1/2}^{n+1} - x_{i-1/2}^{n+1}$

Cell density.: $\rho_{i}^{n+1} = M_{i,\text{cell}} \Big/ V_{i,\text{cell}}^{n+1} \Rightarrow \tau_{i}^{n+1} = 1/\rho_{i}^{n+1}$

Cell SIE: $\varepsilon_{i}^{n+1} = \varepsilon_{i}^{n} - (1/2)(p_{i}^{n+1} + q_{i}^{n+1} - p_{i}^{n} - q_{i}^{n})(\tau_{i}^{n+1} - \tau_{i}^{n})$

Cell pressure: $p_{i}^{n+1} = \mathcal{P}(\varepsilon_{i}^{n+1}, \tau_{i}^{n+1})$ ***Full EOS call***

These are implicit, nonlinear equations in ε_{i}^{n+1} and p_{i}^{n+1} that are solved with an iterative solution procedure.

- **For multiple materials, Alg. II changes similarly to Alg. I**

* Yanilkin, Yu.V., *Study and Implementation of Multi-Material Pressure Relaxation Methods for Lagrangian Hydrodynamics*, Los Alamos National Laboratory report LA-UR-10-06664, 2010.

Algorithm III is similar to the first algorithm*.

Predictor

Edge positions: $x_{i+1/2}^{n+1/2} = x_{i+1/2}^{n} + (\Delta t/2)\, u_{i+1/2}^{n}$

Cell volumes: $V_{i,\text{cell}}^{n+1/2} = x_{i+1/2}^{n+1/2} - x_{i-1/2}^{n+1/2}$

Cell specific vol.: $\tau_i^{n+1/2} = V_{i,\text{cell}}^{n+1/2} \Big/ M_{i,\text{cell}}$

Cell pressure: $p_i^{n+1/2} = p_i^n - \left((c_{s,i}^n)^2 \Big/ \tau_i^n\right)\left(\delta V_i^{n+1/2} \Big/ V_i^n\right)$

Adiabatic update

Corrector

Edge-velocities: $u_{i+1/2}^{n+1} = u_{i+1/2}^{n} - \dfrac{\Delta t}{M_{i+1/2,\text{node}}}\left(p_i^{n+1/2} + q_i^{n+1/2} - p_i^{n+1/2} - q_i^{n+1/2}\right)$

Edge positions: $x_{i+1/2}^{n+1} = x_{i+1/2}^{n} + \Delta t\left(u_{i+1/2}^{n} + u_{i+1/2}^{n+1}\right)/2$

Cell volumes: $V_{i,\text{cell}}^{n+1} = x_{i+1/2}^{n+1} - x_{i-1/2}^{n+1}$

Cell specific vol.: $\tau_i^{n+1} = V_{i,\text{cell}}^{n+1} \Big/ M_{i,\text{cell}}$

Cell SIE: $\varepsilon_i^{n+1} = \varepsilon_i^{n} - \left(\left(p_i^{n+1} + q_i^{n+1}\right)\delta V_i^{n+1} \Big/ M_{i,\text{cell}}\right)$

Cell pressure: $p_i^{n+1} = \mathcal{P}(\varepsilon_i^{n+1}, \tau_i^{n+1})$

Artificial viscosity

* Kamm J.R., Shashkov M.J., Rider, W.J., "A new pressure relaxation closure model for one-dimensional two-material Lagrangian hydrodynamics, *Eur. Phys. J. Web Conf.* 2011, doi:10.1051/epjconf/201010000038.

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With Alg. I, several closure models for pressure equilibration can be examined.

① **Equal compressibility***: $\nabla\cdot u_\alpha = \nabla\cdot u$ **so** $\lambda_\alpha = 1,\ \psi_\alpha = f_\alpha$

- Assume this is valid at the predictor step: $\nabla\cdot u_\alpha^{n+1/2} = \nabla\cdot u^{n+1/2}$
- Easy to implement; computationally efficient: $p = \Sigma\, f_\alpha\, p_\alpha$
- Physically incorrect—with questionable results—in many situations.
  - E.g., cell with gas (highly compressible) and metal (low compressibility).

② **Equal pressure**†: $p_1 = p_2$ **and** $q_1 = q_2$

- This is the result of instantaneous (i.e., over Δt) pressure equilibration.
- Leads to coupled equations: one must solve for $\Delta E_\alpha,\ \Delta V,\ p^{n+1/2}$ in:

$$\Delta E_\alpha = (p^{n+1/2}+q^n)\ \mu\ \Delta V_\alpha\ ,\quad \Delta V = \Sigma\ \Delta V_\alpha\ ,\quad p^{n+1/2} = \mathcal{P}\left(\frac{M_\alpha}{V_\alpha^n+\Delta V_\alpha}, \frac{E_\alpha+\Delta E_\alpha}{M_\alpha}\right)$$

where $\mu \equiv (\nabla\cdot u^n + \nabla\cdot u^{n+1})V^n\Delta t/(2\Delta V)$

- These imply expressions for updated SIE and volume fraction:

$$\varepsilon_\alpha^{n+1/2} = \varepsilon_\alpha + (\Delta E_\alpha/M_\alpha)\ ,\quad f_\alpha^{n+1/2} = (V_\alpha+\Delta V_\alpha)/(V+\Delta V)$$

- Bakhrakh, S., Spiridonov, V., Shanin, A., "A method for computing gas-dynamic flows of inhomogeneous medium in Lagrangian-Eulerian coordinates," *DAN SSR* 1984;**276**:829–833 (in Russian; translated in *Sov. Phys. Doklady* 1984;**29**:443–445).

† Harlow, F., "The particle-in-cell computing method for fluid dynamics," in Alder, B., Fernbach, S., Rotenberg, M., eds., *Methods in Computational Physics*, Vol. 3; New York: Academic Press; 1964, 319–343; Zharova, G.V., Yanilkin, Yu.V. "The EGAK code mixed cell pressure equilibration algorithm," *VANT (Mathematical Modeling of Physical Processes)* 1993;**3**:77–81 (in Russian).

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Equal-increment models can also be formulated.

③ Equal pressure increments* (ΔP):

- Assume that the general acoustic approximation is valid:

$$\partial P/\partial t = (\partial P/\partial \rho)(\partial \rho/\partial t) = \rho\, c^2\, \nabla\cdot u$$

- Assume that this quantity has the same value for all materials:

$$\rho_1 c_1^2\ \nabla\cdot u_1 = \rho_2 c_2^2 \nabla\cdot u_2$$

- This leads to the following closed-form expressions:

$$\nabla\cdot u_\alpha^n = \lambda_\alpha \nabla\cdot u^n \qquad \text{where} \qquad \lambda_\alpha \equiv \frac{1}{\rho_\alpha^n (c_\alpha^n)^2}\left(\sum \frac{f_\beta^n}{\rho_\beta^n (c_\beta^n)^2}\right)^{-1}$$

④ Equal velocity increments† (Δv):

- One velocity per cell, so equal velocity *increments* is plausible.
- Acoustic approximation implies: $\nabla\cdot u_\alpha \approx -(\delta\rho_\alpha)/(\rho_\alpha \Delta t) \approx -(\delta u_\alpha)/(c_\alpha \Delta t)$
- This leads to the following closed-form expressions:

$$\nabla\cdot u_\alpha^n = \lambda_\alpha \nabla\cdot u^n \qquad \text{where} \qquad \lambda_\alpha \equiv \frac{1}{c_\alpha^n}\left(\sum (f_\beta^n / c_\beta^n)\right)^{-1}$$

- Bondarenko, Yu.A., Yanilkin, Yu.V., "Computation of thermodynamical parameters of the mixed cells in gas dynamics," *VANT* (*Mathematical Modeling of Physical Processes*) 2000;**4**:12–25 (in Russian).

† Goncharov, E.A., Yanilkin, Yu.V., "New method for computations of thermodynamical states of the materials in mixed cells," *VANT* (*Mathematical Modeling of Physical Processes*) 2004;**3**:16–30 (in Russian).

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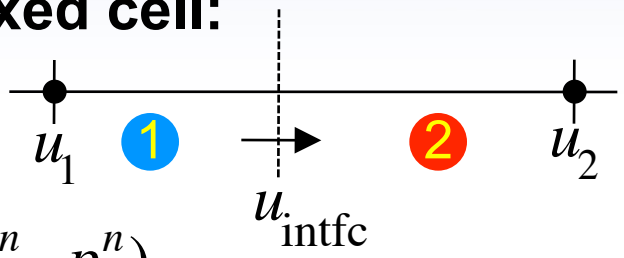
With Alg. II, a linearized Riemann problem* (LRP) used.

⑤ Consider a Riemann problem in the mixed cell:

- Riemann invariants imply the well-known linearized contact velocity expression:



$$u_{\text{intfc}}^{n+1/2} = \frac{(\rho c_s)_1^n u_1^{n+1/2} + (\rho c_s)_2^n u_2^{n+1/2} + (p_1^n - p_2^n)}{(\rho c_s)_1^n + (\rho c_s)_2^n}$$

- From Algorithm II, the following update for the density follows:

$$\frac{1}{\rho^{n+1}} - \frac{1}{\rho^n} = \Delta t^+ \frac{u_i^{n+1/2} - u_{i-1}^{n+1/2}}{M}$$

- Combining these equations gives updates for each material implies:

$$\frac{1}{\rho_1^{n+1}} - \frac{1}{\rho_1^n} = \frac{\Delta t}{M_1}\left[\frac{(\rho c_s)_2^n}{(\rho c_s)_1^n + (\rho c_s)_2^n}(u_i^{n+1/2} - u_{i-1}^{n+1/2}) + \frac{p_1^n - p_2^n}{(\rho c_s)_1^n + (\rho c_s)_2^n}\right]$$

$$\frac{1}{\rho_2^{n+1}} - \frac{1}{\rho_2^n} = \frac{\Delta t}{M_2}\left[\frac{(\rho c_s)_1^n}{(\rho c_s)_1^n + (\rho c_s)_2^n}(u_i^{n+1/2} - u_{i-1}^{n+1/2}) - \frac{p_1^n - p_2^n}{(\rho c_s)_1^n + (\rho c_s)_2^n}\right]$$

- Delov, V., Sadchikov, V.V., "Comparison of several models for computation of thermodynamical parameters for heterogeneous Lagrangian cells," *VANT (Mathematical Modeling of Physical Processes)* 2005;**1**:57–70 (in Russian).

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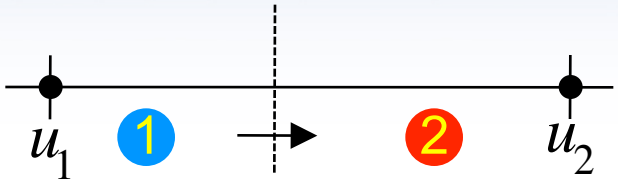
The LRP* method also involves additional equations.

- From $\nabla\cdot u \approx \Delta V/(V\Delta t)$, the individual velocity divergences are obtained:



$$\nabla\cdot u_\alpha^n = (\lambda_\alpha / f_\alpha^n)\nabla\cdot u^n + \omega^n\left[(p_\alpha^n - p_\Sigma^n)/(f_\alpha^n h^n)\right]\cdot\left[(\rho c)_\Sigma^n\right]^{-1}$$

where

$$p_\Sigma^n \equiv \tfrac{1}{2}(p_1^n + p_2^n)\ , \qquad (\rho c)_\Sigma^n \equiv \tfrac{1}{2}\left[(\rho c)_1^n + (\rho c)_2^n\right]\ , \qquad \lambda_\alpha \equiv 1 - \left[\tfrac{1}{2}(\rho c)_1^n/(\rho c)_\Sigma^n\right]\ ,$$

with h^n a characteristic mesh size and ω^n improves stability:

$$\omega^n \equiv \left\{\tfrac{1}{2}\left[(\rho c)_1^n + (\rho c)_2^n\right]\right\}^2 \left\{\rho^n\left[(\rho c^2)_1^n + (\rho c^2)_2^n\right]\right\}^{-1} \min\left\{f_1^n, f_2^n\right\}$$

- From the velocity divergence equation, the volume change is:

$$V_\alpha^{n+1} - V_\alpha^n = \lambda_\alpha (V^{n+1} - V^n) + (\omega\,\Delta t\, V^n/h)\,(p_\alpha^n - p_\Sigma^n)\left[(\rho c)_\Sigma^n\right]^{-1}$$

- After some algebra, this implies that the energy update for material α is modified by an additional term:

$$\Delta\varepsilon_\alpha^{n+1} = \left[(\omega^n\tau)/(\rho^n h^n)\right] f_\alpha \left[p_1^n(p_1^n - p_\Sigma^n) + p_2^n(p_2^n - p_\Sigma^n)\right]\left[(\rho c)_\Sigma^n\right]^{-1}$$

- Delov, V., Sadchikov, V.V., "Comparison of several models for computation of thermodynamical parameters for heterogeneous Lagrangian cells," *VANT (Mathematical Modeling of Physical Processes)* 2005;**1**:57–70 (in Russian).

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Kamm & Shashkov* (KS) break the pressure equilibration assumption of Després† using local Riemann problem solutions.

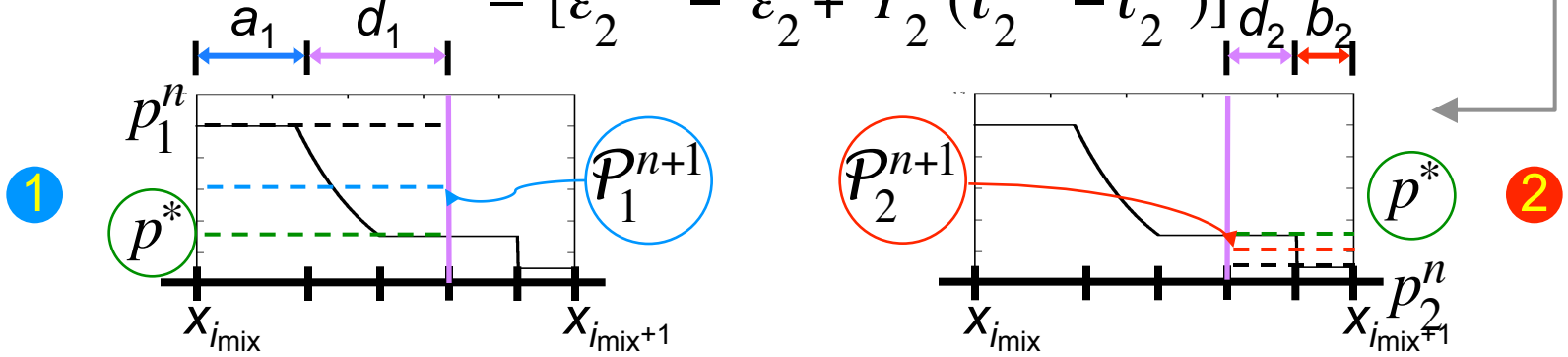
- Pressure relaxation in the mixed cell reduces to the solution of a minimization problem in τ_1^{n+1}, ε_1^{n+1}, τ_2^{n+1}, ε_2^{n+1}

$$\min_{\{\tau_1^{n+1},\varepsilon_1^{n+1},\tau_2^{n+1},\varepsilon_2^{n+1}\}} f_0 \equiv \|\mathcal{P}_1^{n+1} - p_1^{RP}\| + \|\mathcal{P}_2^{n+1} - p_2^{RP}\|$$

subject to:

$$\begin{aligned} 0 &= f_1 \equiv c_1\,\tau_1^{n+1} + c_2\,\tau_2^{n+1} - \tau^{n+1} \\ 0 &= f_2 \equiv c_1\,\varepsilon_1^{n+1} + c_2\,\varepsilon_2^{n+1} - \varepsilon^{n+1} \\ 0 &= f_3 \equiv \varepsilon_1^{n+1} - \varepsilon_1^{n} + P_1\,(\tau_1^{n+1} - \tau_1^{n}) \\ &\quad - [\varepsilon_2^{n+1} - \varepsilon_2^{n} + P_2\,(\tau_2^{n+1} - \tau_2^{n})] \end{aligned}$$

Mixed-cell Riemann Problem

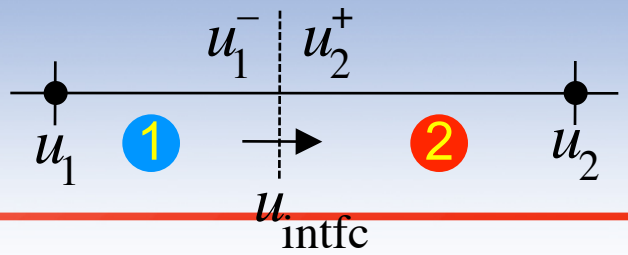


- Complicated — and untested for realistic problems in multi-D.

• Kamm J.R., Shashkov M.J., *Comm. Comput. Phys.*, 2010; **7**:927–976.

† Després, B., Lagoutière, F., *Prog. Comput. Fluid Dyn.* 2007; **7**:295–310.

Kamm, Shashkov & Rider* (KSR) also propose a linearized Riemann model.



- Inspired by VNIIEF work, KSR used the linearized Riemann problem to update the materials' volumes, volume fractions, and SIEs.
- There is a problem: this SIE update is *not consistent* with the total work done on the mixed cell, i.e., $\sum_k M_k \, d\varepsilon_k^{n+1,*} \neq -p_{i_{\text{mix}}+1/2}^{n+1/2} \, dV_{i_{\text{mix}}+1/2}^{n+1}$
- Let $d\tilde{\varepsilon}_k$ be the change in SIE that guarantees consistency:

Consistent $\varepsilon_k^{n+1} = \varepsilon_k^{n+1,*} + d\tilde{\varepsilon}_k$ *Known* + *Unknown*

- Assume that the pressure change due to $d\tilde{\varepsilon}_k$: (1) is the same for both materials, and (2) depends *only* on the energy (*not* on the density).
- Using the expression for the total SIE discrepancy and the thermodynamic derivatives $\left(\partial p_k / \partial \varepsilon_k\right)_{\rho_k}$, one can solve for the corrections to the SIEs and then update the pressures:

$$\varepsilon_k^{n+1} = \varepsilon_k^{n+1,*} + d\tilde{\varepsilon}_k \quad \text{and} \quad p_k^{n+1} = \mathcal{P}_k(\varepsilon_k^{n+1}, \tau_k^{n+1})$$

• Kamm J.R., Shashkov M.J., Rider, W.J., "A new pressure relaxation closure model for one-dimensional two-material Lagrangian hydrodynamics, *Eur. Phys. J. Web Conf.* 2011, doi:10.1051/epjconf/201010000038.

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Tipton's method is a widely used, robust multi-material, pressure relaxation for multi-D.

- Assumption #1: Predictor pressure based on adiabatic update:

$$p_k^{n+1/2} = p_k^n - \left[\left(cs_k^n\right)^2 \Big/ \tau_k^n\right]\left(\boxed{\delta V_k^{n+1/2}} \Big/ V_k^n\right)$$

Unknown

- Assumption #2: There is a relaxation term added to each material's pressure, so that these sums are all equal:

Unknown

Predictor pressure of k-th material $p_k^{n+1/2} + \boxed{R_k} = \boxed{\hat{p}^{n+1/2}}$ *Overall predictor pressure*

where $\boxed{R_k} = -\left(cs_k^n \Big/ \tau_k^n\right)\left(L^n \Big/ \delta t\right)\left(\boxed{\delta V_k^{n+1/2}} \Big/ V_k^n\right)$ *Relaxation term for k-th material*

- Assumption #3: Volume changes add up correctly:

$$\sum_k \boxed{\delta V_k^{n+1/2}} = V^{n+1/2}$$

Total predictor volume change is known from standard algorithm

- One can solve for $\hat{p}^{n+1/2}$ and $\delta V_k^{n+1/2}$ in closed form.
- The second step of a two-step time-integrator uses this information to obtain the final updated values.

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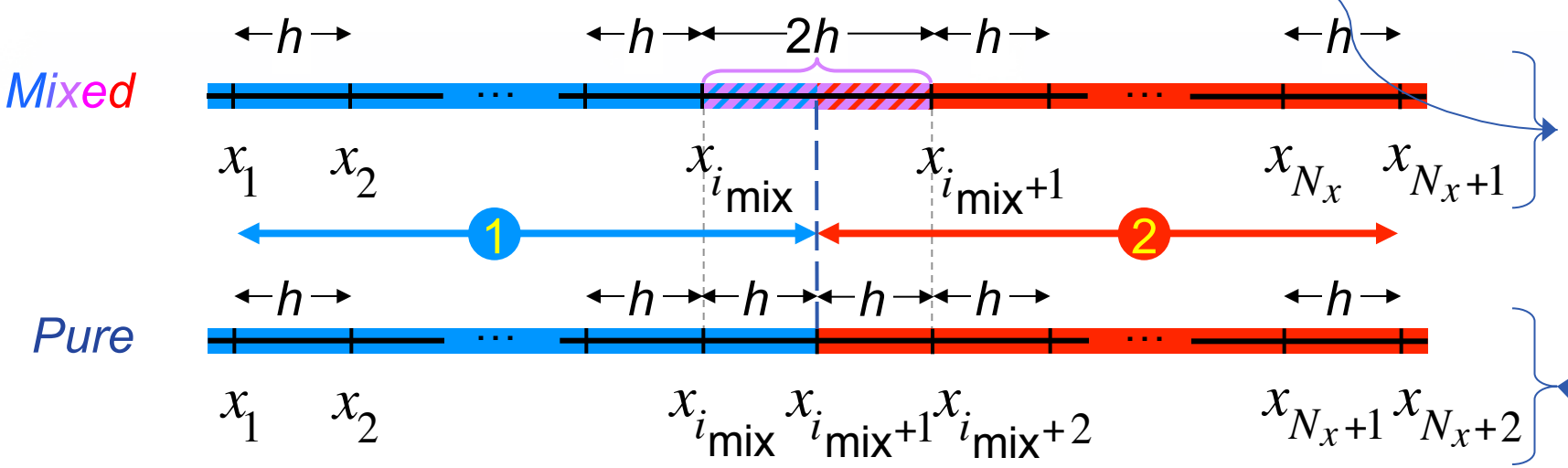
The initialization of the pure-material and mixed-cell test problems are as follows.

- **The test problems were run similarly:**
  - N_x zones on $x_{\min} \le x < x_{\max}$ with $\Delta x_i = h$, $i \ne i_{\text{mix}}$
  - One mixed cell for $i = i_{\text{mix}}$ with $\Delta x_{i_{\text{mix}}} = 2h$



- The fictitious mixed-cell interface is at the center of mixed cell of width 2*h*, with no explicit mass-matching.
- We compare these results with pure-material calculations that have the actual interface.

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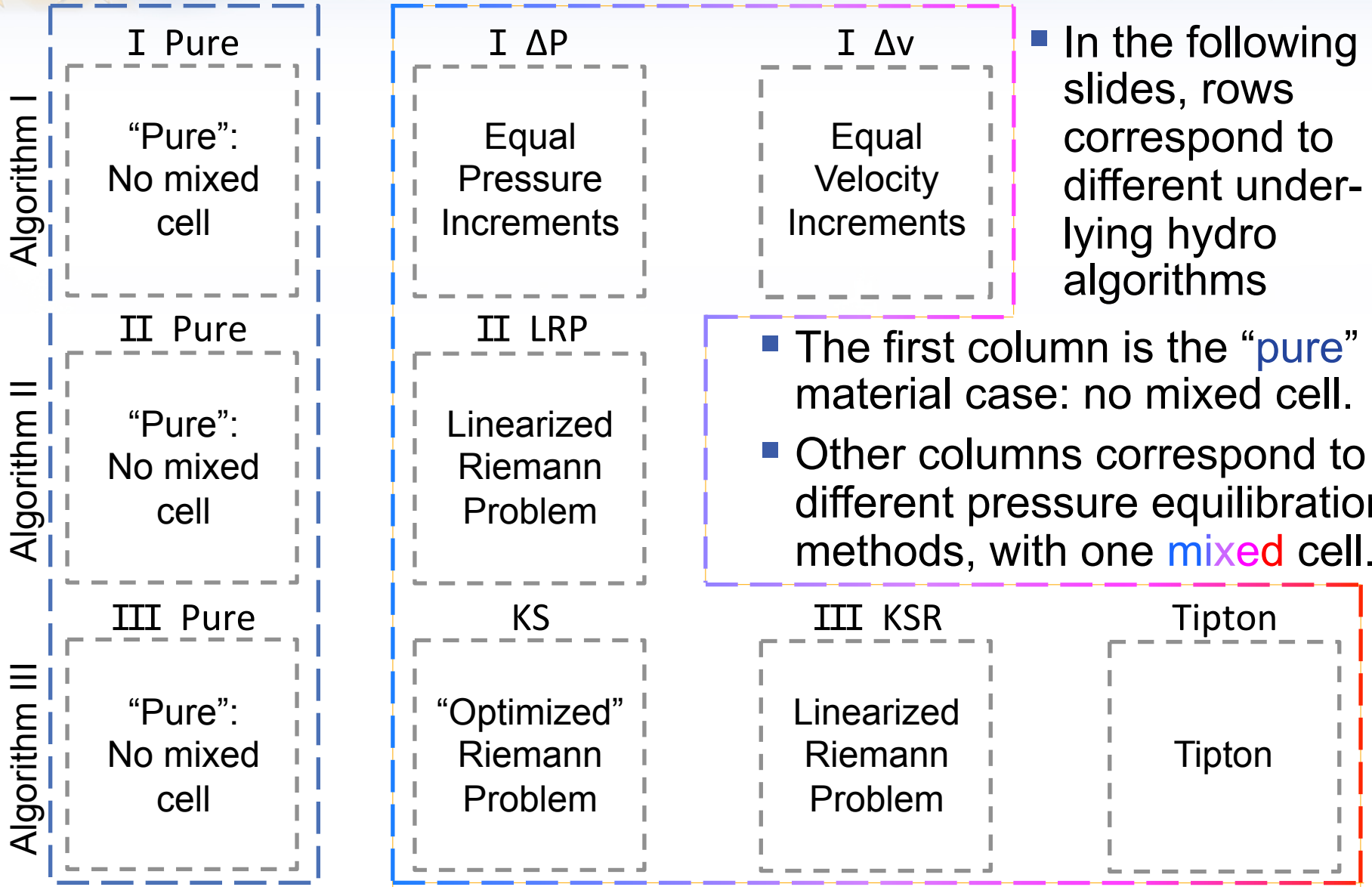
The template for the test problem time-history results is as follows.



- In the following slides, rows correspond to different under-lying hydro algorithms
  - The first column is the "pure" material case: no mixed cell.
  - Other columns correspond to different pressure equilibration methods, with one mixed cell.

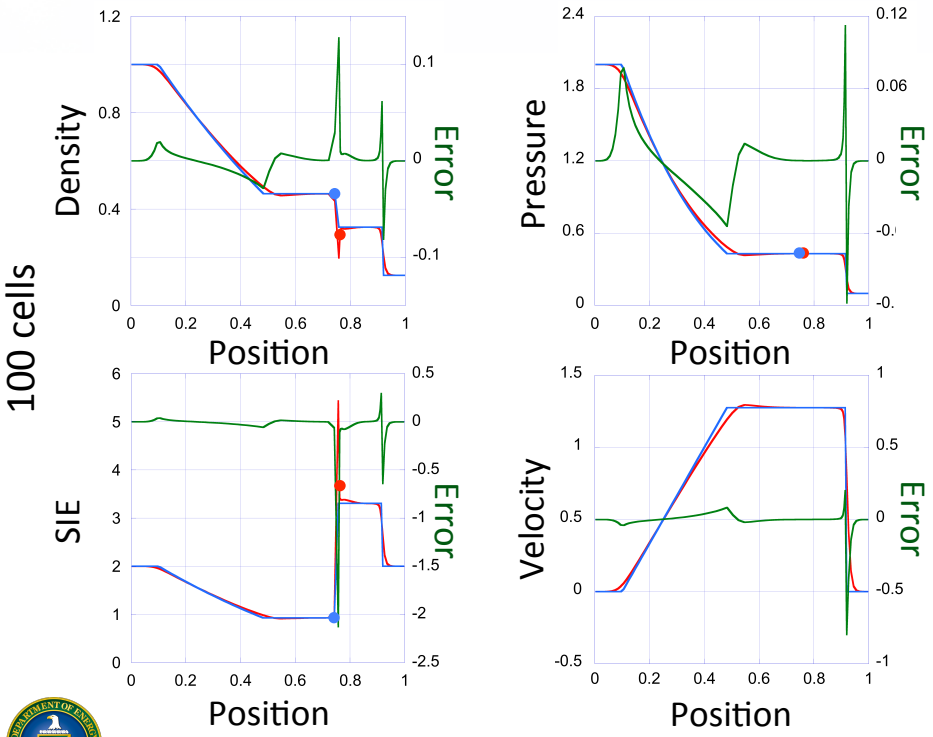
*Tufte, E., *The Visual Display of Quantitative Information*, Graphics Press, Cheshire, CT, 2007.

Test Problem #1: Modified Sod Shock Tube

- Modified Sod initial conditions:

$$(\rho, p, u, \gamma) = \begin{cases} (1.0, \quad 2.0, 0.0, 2.0), & 0 \le x < 0.5, \text{ Material 1} \\ (0.125, 0.1, 0.0, 1.4), & 0.5 < x \le 1.0, \text{ Material 2} \end{cases} \qquad t_{\text{final}} = 0.2$$

- Final-time snapshots show the standard shock-tube evolution.



"Closed-form" – Computed = Error

- In the following slides, we present time-histories in the single mixed cell.
- Results for all of the methods mentioned are presented.
  - All methods have been demonstrated to be about first-order accurate on this problem.

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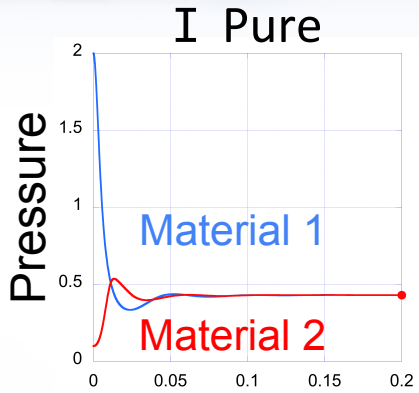
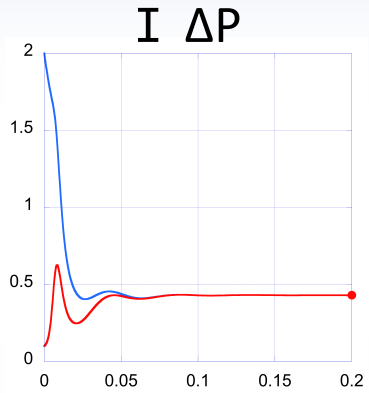
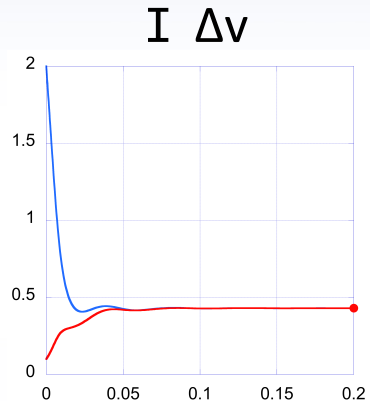
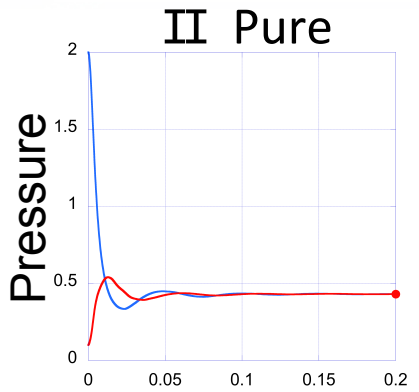
Modified Sod Pressure History

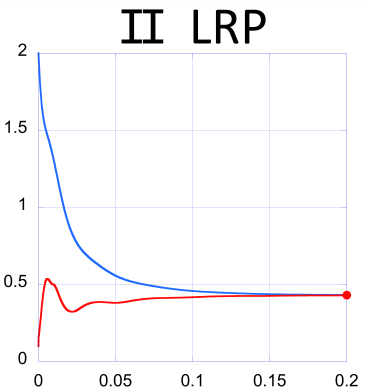




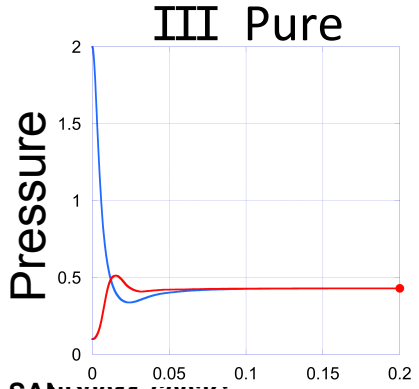


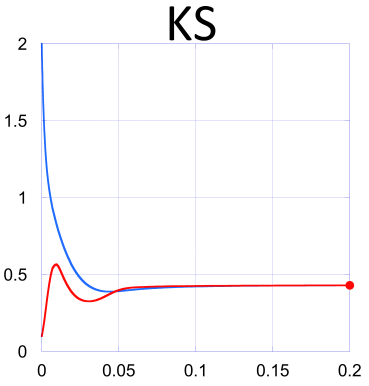
- All methods:
  - Equilibrate
  - Obtain the correct final pressure

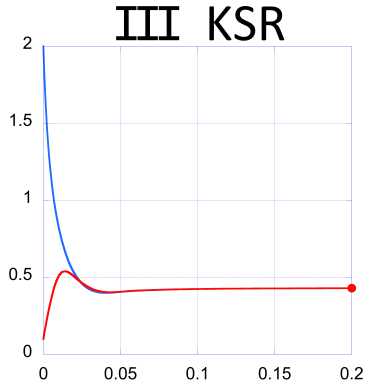


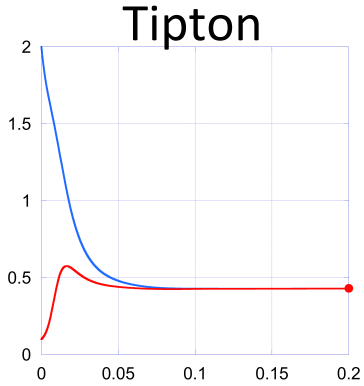


- All methods exhibit pressure oscillations, also.
- Among mixed cell methods, KSR and Tipton look heuristically the “nicest.”

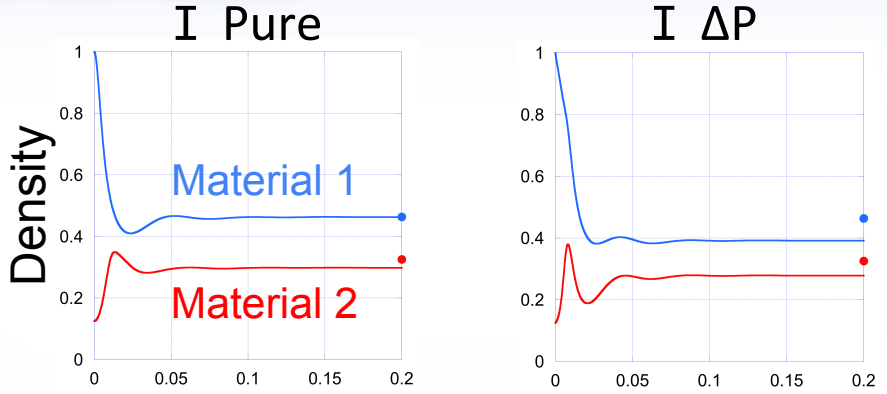


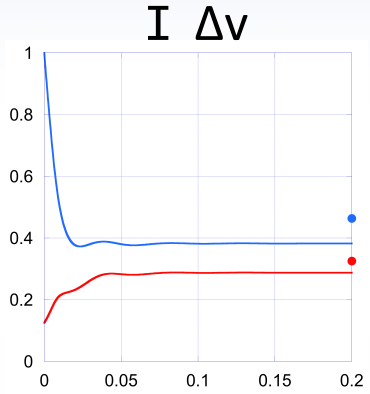




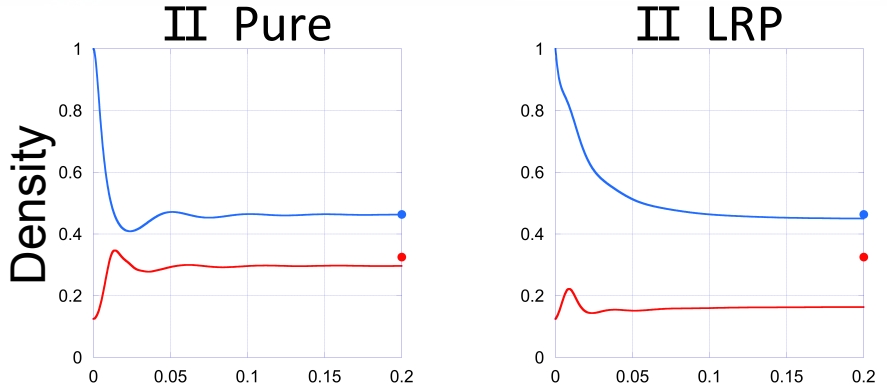


Modified Sod Density History

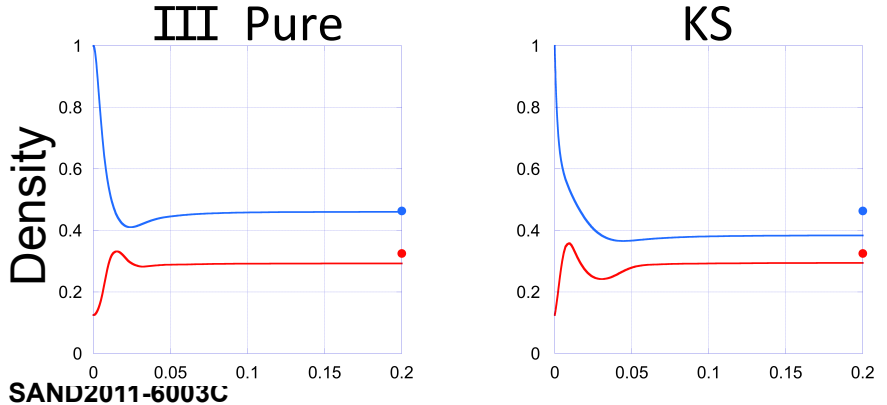


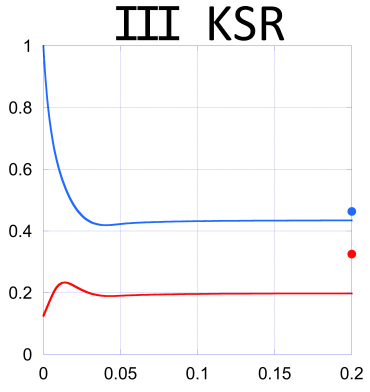


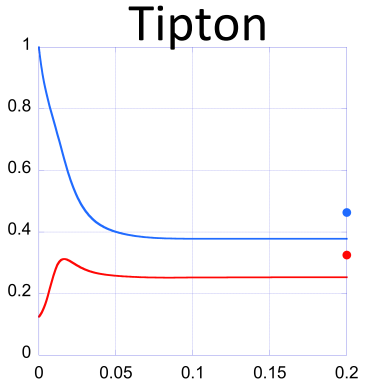
- The "pure" methods come closest to the correct values at the final time.



- All mixed cell methods undershoot the final values.
- Which method looks heuristically the "best"?







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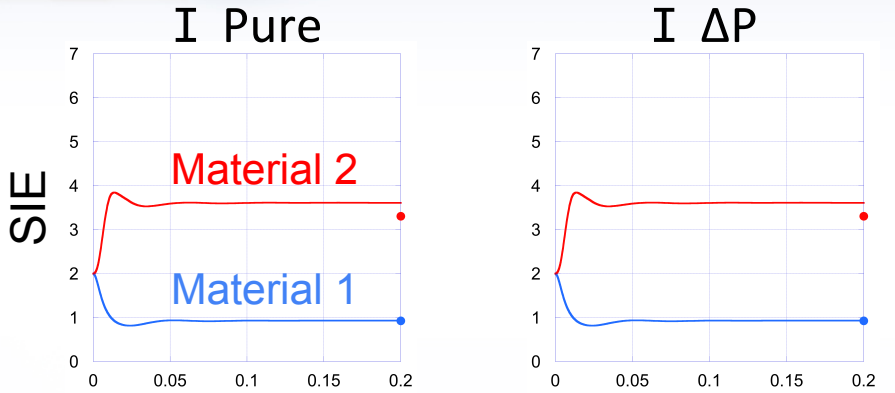
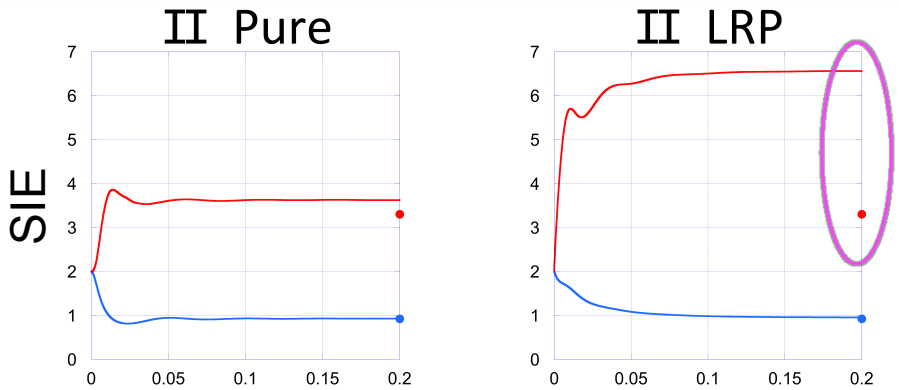
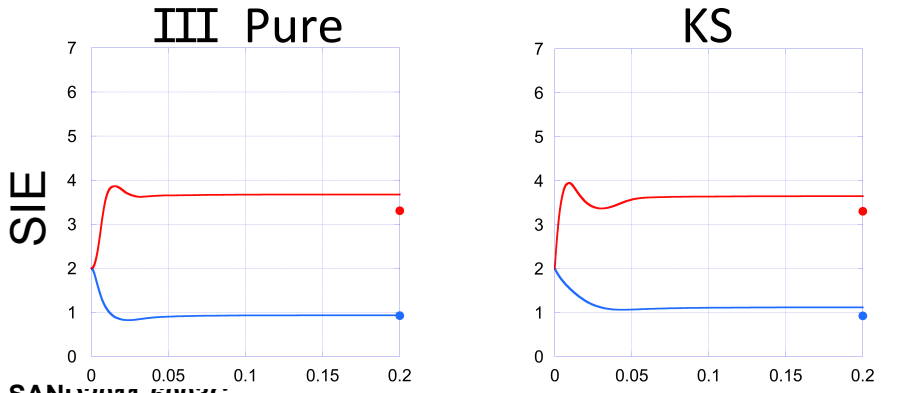
Modified Sod Specific Internal Energy History







- For material 1, all methods perform about equally well, and get the correct result.
- For material 2, both linearized Riemann problem methods overshoot significantly.
- Tipton overshoots a little, too.
- KS heuristically the “best”?

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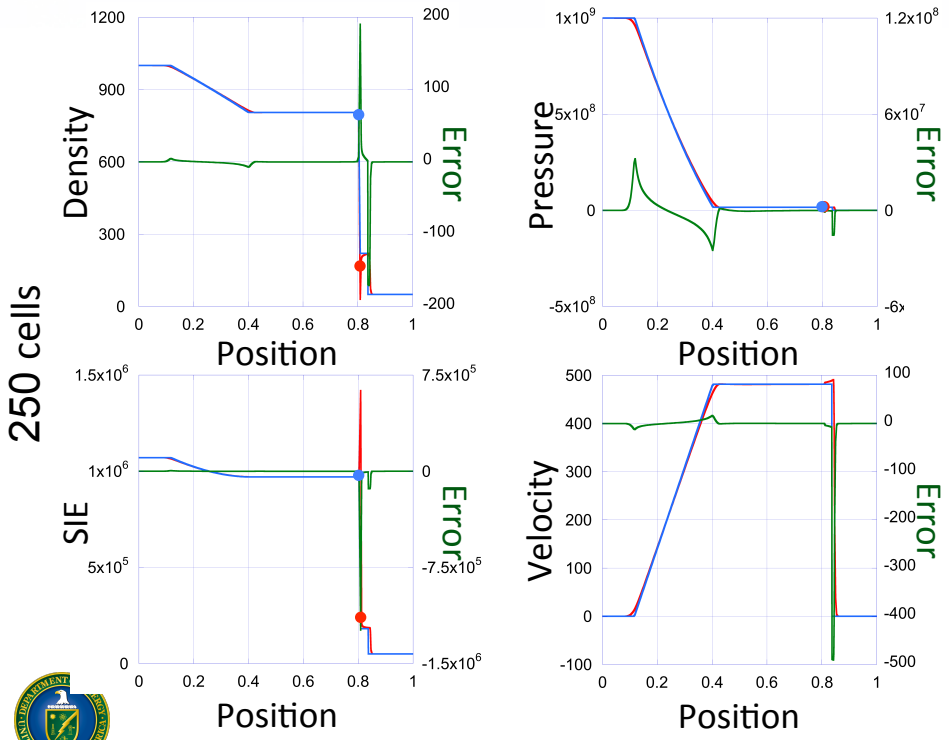
Test Problem #2: the Water-Air Shock Tube

- Water-air shock tube* initial conditions:

$$(\rho, p, u, \gamma, p_\infty) = \begin{cases} (1.e+3, 1.e+9, 0.0, 4.4, 6.e+8), & 0 \le x < 0.7, \text{ Material 1} \\ (5.e+1, 1.e+6, 0.0, 1.4, 0.0), & 0.7 < x \le 1.0, \text{ Material 2} \end{cases} \quad \begin{array}{l} p = (\gamma - 1)\rho\varepsilon - \gamma p_\infty \\ t_{\text{final}} = 2.2\text{e-}4 \end{array}$$

- Final-time snapshots show the stronger shock-tube evolution.



"Closed-form" – *Computed* = *Error*

- In the following slides, we present time-histories in the single mixed cell.
- Results for all of the methods mentioned are presented.
  - All methods have been demonstrated to be about first-order accurate on this problem.

* R. Saurel & R. Abgrall, "A Multiphase Godunov Method for Compressible Multifluid and Multiphase Flows," *J. Comput. Phys.* 1999; **150**:425–467.

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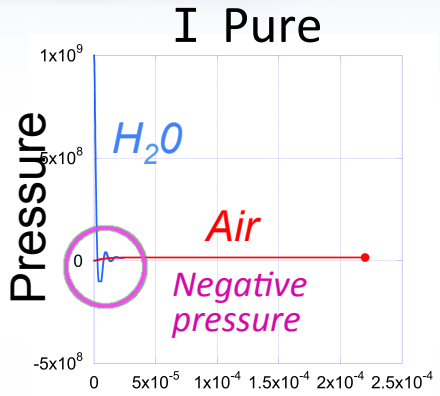
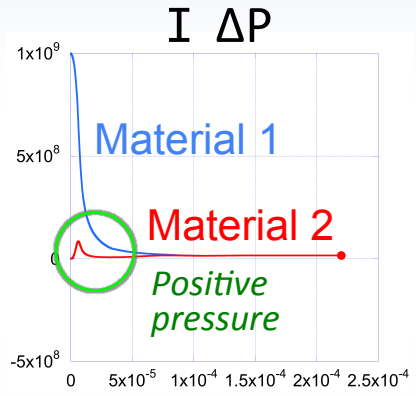
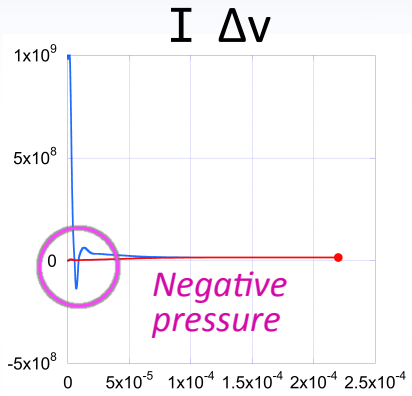
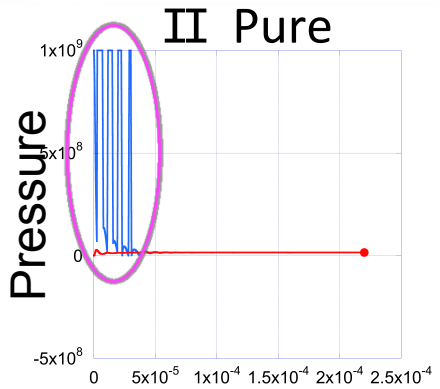
Water-Air Pressure History

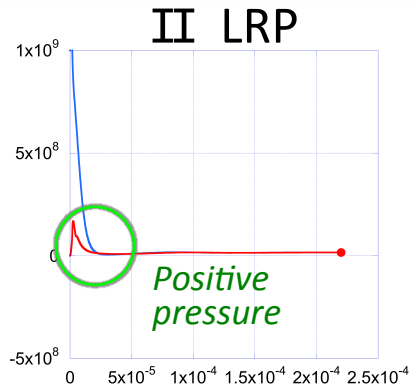




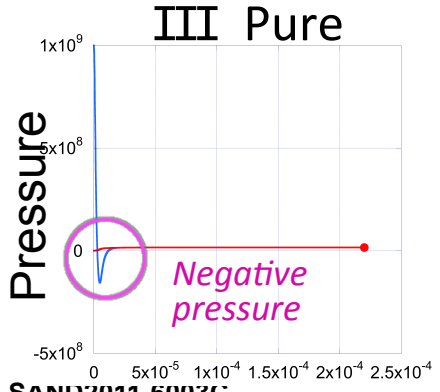


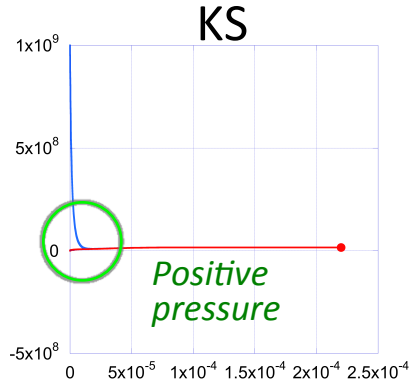
- All methods:
  - Equilibrate
  - Obtain the correct final pressure

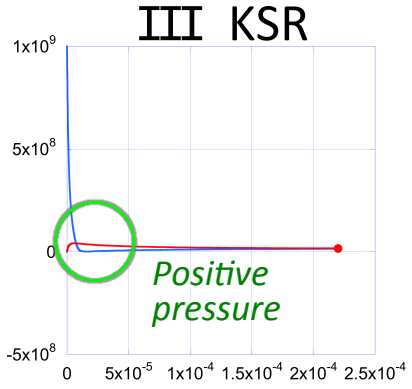


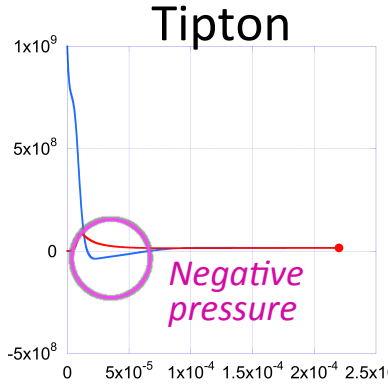


- Some pure and mixed cell methods have negative pressure.
- The mixed cell methods based on Riemann problems have no negative pressure.

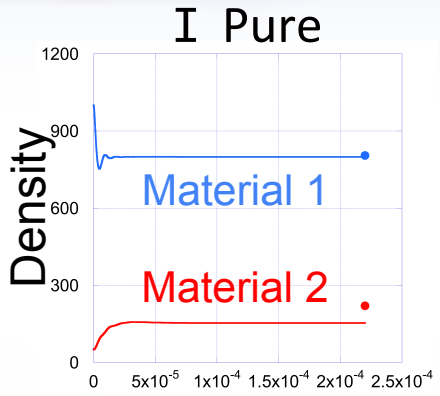


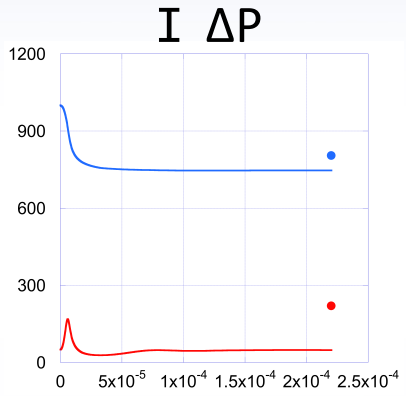


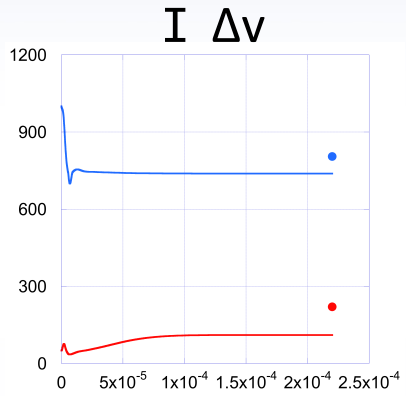




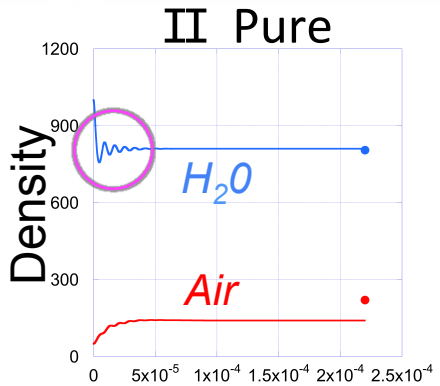
Water-Air Density History

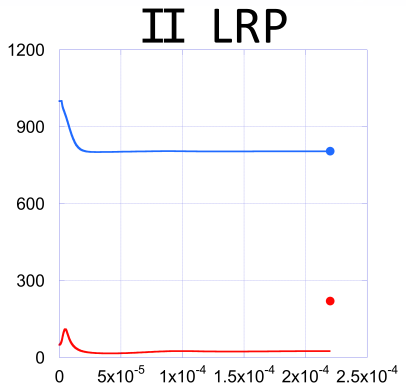




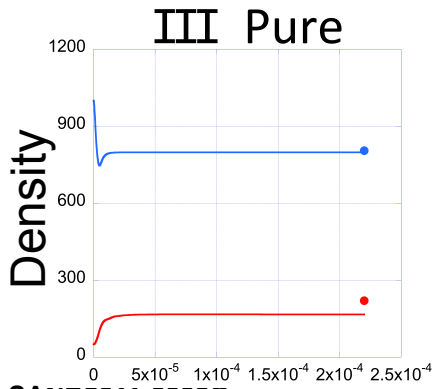


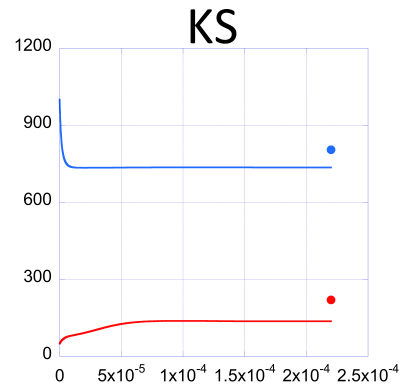
- The "pure" methods come closest to the correct values at the final time.

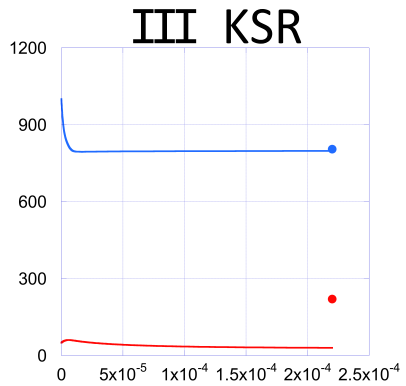


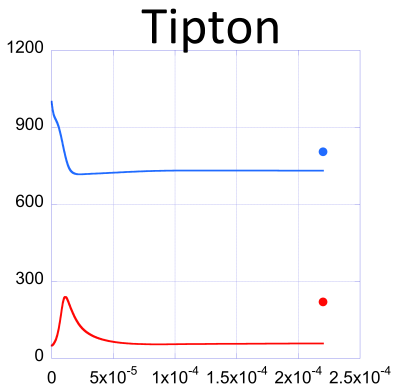


- For material 2, mixed cell methods consistently undershoot final values more than pure methods.
- Which method looks heuristically the "best"?

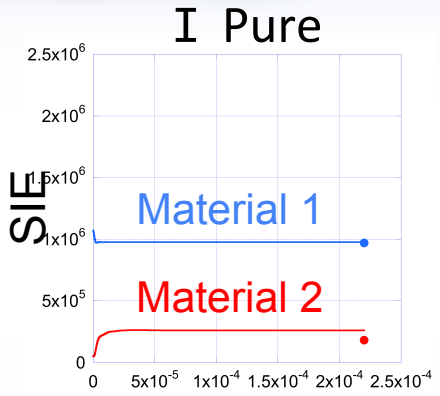


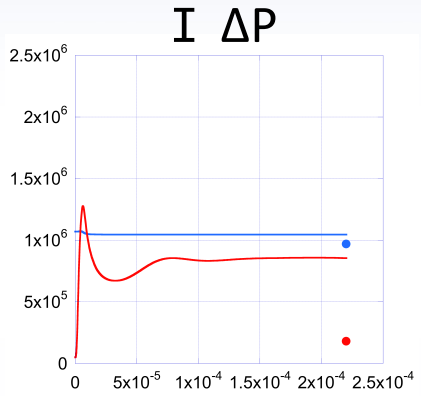


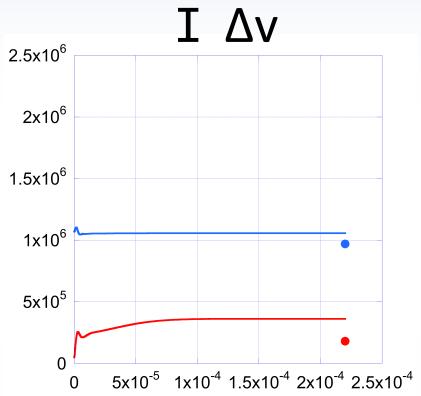




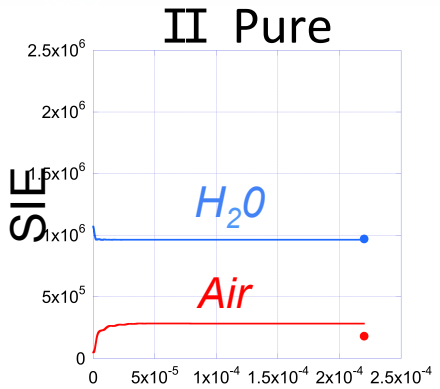
Water-Air Specific Internal Energy History

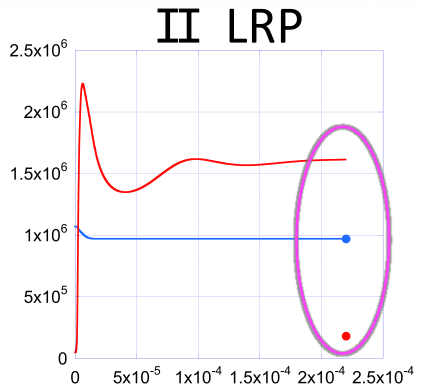




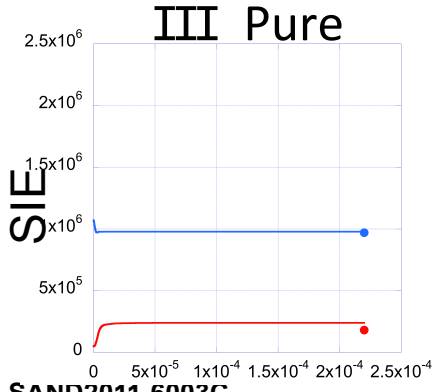


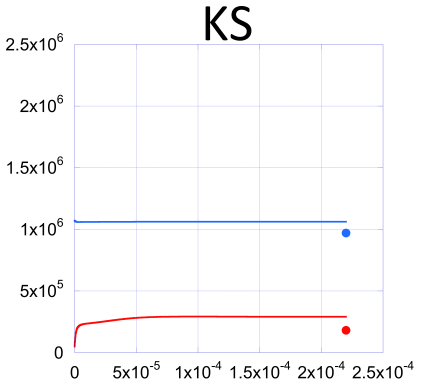
- For material 1, all methods are about the same, close to the exact final value.

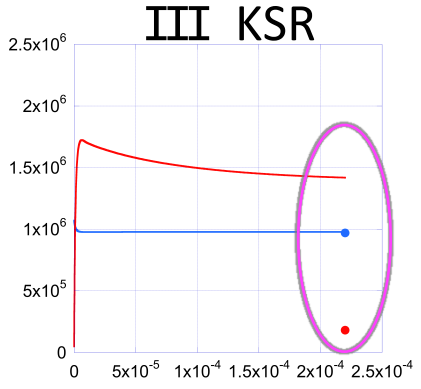


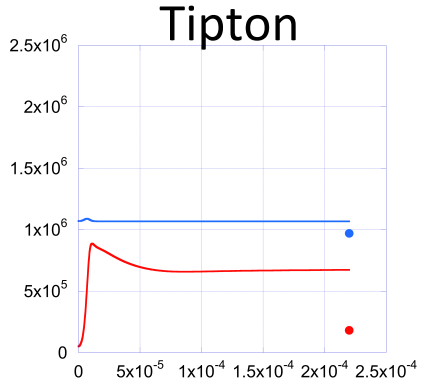


- For material 2, both linearized Riemann problem methods overshoot seriously.
  - Tipton, ΔP overshoot material 2.
  - KSR has volume fraction "flip."









Summary of these results

- **Pure Material:**
  - Basic algorithm with no mixed cell; straightforward for ideal problems.
  - (+) No mixed cell assumptions.
  - (−) No mixed cell assumptions.
- **Equal ΔP:**
  - Acoustic approximation, assumed to be equal for all materials.
  - (+) Closed-form expressions, 2-D.
  - (−) Sometimes oscillatory, less accurate SIE.
- **Equal Δv:**
  - Single velocity → equal velocity increments is a plausible assumption.
  - (+) Closed-form expressions, 2-D.
  - (−) Sometimes oscillatory, negative pressure.
- **Linearized Riemann Problem (LRP):**
  - Linearized Riemann problem in mixed cell is used as conservative closure.
  - (+) "Physics-based", 2-D.
  - (−) Questionable SIE, volume fractions.
- **Kamm & Shashkov (KS):**
  - Full Riemann problem in mixed cell → "optimal" pressure of each material.
  - (+) Physics-based.
  - (−) Complicated. 2-D? Strength?
- **Kamm, Shashkov & Rider (KSR):**
  - Linearized Riemann problem in mixed cell is used as conservative closure.
  - (+) "Physics-based", 2-D.
  - (−) Questionable SIE, volume fractions.
- **Tipton:**
  - Relaxation term → equal pressures: solve *exactly* for this term.
  - (+) Robust, fast, 2-D & strength.
  - (−) Rough & ready assumptions, good results.

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Conclusions

- **Multi-material Lagrangian cells remain an important issue.**
  - The 1-D case allows rigorous testing of closure models.
- **Several different closure models were described.**
  - Some are simple & fast (e.g., equal compressibility), while others are complex & slow (e.g., using the full Riemann problem).
  - Unfortunately, these methods were not all tested with *exactly* the same underlying hydro integration scheme.
- **There is no clear "winner" among the methods**
  - In some aspects, simple methods look good (e.g., ΔP)
  - In other aspects, Riemann-based methods do not (e.g., SIE)
  - Other problems? Strong expansions, stronger shocks, near-void.
- **Many of these approaches can be extended:**
  - ≥ 2 materials, with some assumptions about material ordering.
  - 2-D and 3-D: VNIIEF methods (Yanilkin et al.) and KSR (Harrison et al.).
- **Open issues: (1) 2-D comparisons? (2) Entropy...**

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